Hall resistance and Lorentz ratio models in YBa$_2$Cu$_3$O$_7$

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Two-dimensional models of heat capacity, conductivity (κ), Hall resistance (R_H) and the Lorentz ratio ($\mathcal{L}$) have been derived using the ionization energy (E_I) based Fermi-Dirac statistics (iFDS) for overdoped Cuprates. These models reproduce the experimentally measured $\rho(T)$ and $R_H(T)$. The variation of $\mathcal{L}$ is weakly T-dependent due to the experimental $\kappa(T)$. The e-ph coupling in the electrical resistivity has the polaronic effect that complies with iFDS, rather than the e-ph scattering, which satisfies the Bloch-Grüneisen formula. These models are purely Fermi liquid and are not associated with any microscopic theories of high-T_c superconductors.

1. Introduction

The electrical properties of high-T_c Cuprate superconductors (HTSC) are intrinsically enigmatic in both experimental and theoretical framework compared to other oxide compounds, including manganites. Partly due to its huge potential in a wide variety of applications, intense focus is given on the nature of conductivity of these materials to shed some light on the puzzling temperature-dependence issues in heat capacity ($\mathcal{C}$), heat conductivity, resistivity, Hall resistance and Lorentz ratio. The conflict in term of T-dependency between ρ and R_H is also one of the unsolved mystery in HTSC. Even though this paper does not solve it microscopically, but it points out that the Fermi liquid with strong correlations is not downright incorrect, at least for over- and optimally doped HTSC. Apart from HTSC, the applications of ionization energy (E_I) based Fermi-Dirac statistics (iFDS) on ferromagnets, diluted ferromagnetic semiconductors and doped ferroelectrics have been derived and discussed analytically [1, 2, 3, 4, 5, 6, 7]. The iFDS in HTSC have been successfully exploited [1, 2, 3] via the experimental data reported in the Refs. [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. Recently, the said puzzling T dependencies as well as the spin gap phenomenon have been tackled with the coupling of iFDS and charge spin separation [20, 21, 22]. Unfortunately, the pure charge-spin separation, is believed to have serious shortcomings [23, 24, 25, 26, 27]. In addition, there are also numerous experimental reports with controversial interpretations surrounding the spin Pseudogap phenomenon [22, 28, 29, 30, 31, 32, 33, 34]. As such, by ignoring the spin Pseudogap phase, the thermo-magneto-electronic properties of YBa$_2$Cu$_3$O$_7$ will be discussed based on the iFDS by heavily relying on the basic transport experiments such as the resistivity, Hall resistance, heat capacity and heat conductivity. It is interesting to note that these purely Fermi-liquid models are able to reproduce the related experimental data reasonably well even if they are only for over- and optimally doped HTSC. The polaronic effect that arises as a result of iFDS is solely due to heavier effective mass effect, which *could* indicate the existence of polarons. But this indication is just an extrapolated assumption since heavy electrons do not necessarily form polarons.

2. Theoretical details

The free-particle Hamiltonian of mass m moving in 3-dimensions is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2. \tag{1}$$

Here, we have make use of the linear momentum operator, $\hat{\mathbf{p}} = -i\hbar\nabla$. Subsequently, one can write the time-independent Schrödinger equation for the same particle, however in an unknown potential, $V(x)$ as

$$-\frac{\hbar^2}{2m}\nabla^2\varphi = (E + V(x))\varphi$$
$$= (E_0 \pm \xi)\varphi. \tag{2}$$

In the second line of Eq. (2), one can notice that the influence of the potential energy on the total energy of that particular particle has been conveniently parameterized as ξ. This energy function, ξ will be characterized later in such a way that one can replace $E + V(x)$ with $E_0 + \xi$ in which, $E_0 = E$ at $T = 0$. Add to that, from Eq. (2), it is obvious that the magnitude of ξ is given by $\pm\xi = E - E_0 + V(x)$. Physically, it implies the energy needed to overcome the potential energy as well as the bound state. Literally, this is exactly what we need to know in any condensed matter, i.e., this magnitude is the one that actually or reasonably defines the properties of the quasiparticles. Subsequently, we obtain

$$\nabla^2 \varphi = -\frac{2m}{\hbar^2}[E_0 \pm \xi]\varphi. \tag{3}$$

$$\frac{\hbar^2 k^2}{2m} = E_0 \pm \xi = \frac{\hbar^2}{2m}[k_0^2 \pm k_\xi^2]. \tag{4}$$

$k^2 = (2m/\hbar^2)[E_0 \pm \xi]$. E and E_0 in a given system range from $+\infty$ to 0 for electrons and 0 to $-\infty$ for holes that eventually explains the $\pm$ sign in ξ. Now, Eq. (2) can be solved to give

$$\varphi = C_N \times$$
$$\exp[i(k_{0,x} \pm k_{\xi,x})x + i(k_{0,y} \pm k_{\xi,y})y + i(k_{0,z} \pm k_{\xi,z})z].$$
$$\varphi_{\mathbf{k}(0,\xi)} = C_N e^{i\mathbf{k}(0,\xi)\cdot\mathbf{r}}. \tag{5}$$

$k^2 = (k_{0,x}^2 \pm k_{\xi,x}^2) + (k_{0,y}^2 \pm k_{\xi,y}^2) + (k_{0,z}^2 \pm k_{\xi,z}^2)$. By employing the orthonormality and Plancherel's theorem, one can find the normalization constant, C_N by comparing Eqs. (6) and (7) as shown below.

$$\langle \varphi_{\mathbf{k}_0} \mid \varphi_{\mathbf{k}_0 \pm \mathbf{k}_\xi} \rangle = \int \int \int \varphi_{\mathbf{k}_0} * \varphi_{\mathbf{k}_0 \pm \mathbf{k}_\xi} dx dy dz$$
$$= C_N^2 \int \int \int e^{i[\mathbf{k}_0 - (\mathbf{k}_0 \pm \mathbf{k}_\xi)]\cdot\mathbf{r}} dx dy dz$$
$$= \delta(\mp \mathbf{k}_\xi). \tag{6}$$

$$\frac{1}{(2\pi)^3} \int \int \int e^{i\mathbf{k}_0\cdot(\mathbf{r}-\mathbf{r}')} dk_x dk_y dk_z = \delta(\mathbf{r}-\mathbf{r}'). \tag{7}$$

Hence, $C_N = 1/(2\pi)^{3/2}$. finally, the normalized wave function, which corresponds to Eq. (2) is

$$\varphi_{\mathbf{k}(0,\xi)} = \frac{1}{(2\pi)^{3/2}} e^{i[\mathbf{k}(0,\xi)]\cdot\mathbf{r}}. \tag{8}$$

In a physical sense as stated earlier, $\xi = E - E_0 + V(x)$, is in an identical scale with the energy needed to free an electron from an atom in a given crystal. As such, we apply the concept of ionization energy where, $\xi = E_I^{real}$ $= E_I + V(x)$, to justify that an electron to occupy a higher state N from initial state M is more probable than from initial state L if condition $E_I(M) < E_I(L)$ at certain T is satisfied. As for a hole to occupy a lower state M from initial state N is more probable than to occupy state L if the same condition above is satisfied. It is well known that the exact values of E_I are known for an isolated atom. In this case (for an isolated atom), E_I can be evaluated with

$$E_I = \sum_i^z \frac{E_{Ii}}{z}. \tag{9}$$

However, substituting the same atom in a crystal gives rise to the influence of $V(x)$ and in reality, E_I^{real} cannot be evaluated from Eq. (9). Nevertheless, the E_I^{real} of an atom or ion in a crystal is proportional to the isolated atom and/or ion's E_I as written below.

$$E_I^{real} = \alpha \sum_i^z \frac{E_{Ii}}{z}$$
$$= \alpha E_I. \tag{10}$$

It is this property that enables one to predict the variation of electronic properties of superconductors with substitution reasonably well. The constant of proportionality, α is a function of averaged $V(x)$ and varies with different background atoms. For example, in $YBa_{1-x}Ca_x Cu_2 O_7$ system, YBa_{1-x}-$Cu_2 O_7$ defines the background atoms or ions. Therefore, one needs to employ the experimental data to determine the magnitude of $\xi = E_I^{real} = E_I + V(x)$.

Recall that Eq. (4) simply implies that the one-particle energies E_1, E_2, ..., E_m for the corresponding one-particle quantum states q_1, q_2, ..., q_m can be rewritten as $(E_0 \pm E_I)_1$, $(E_0 \pm E_I)_2$, ..., $(E_0 \pm E_I)_m$. It is also important to note that $E_0 + E_I = E_{electrons}$ and $E_0 - E_I = E_{holes}$. As such, for n particles, the total number of particles and its energies are conserved and the conditions to fulfill those conservations are given by

$$\sum_i^\infty n_i = n, \qquad \sum_i^\infty dn_i = 0. \tag{11}$$

$$\sum_i^\infty (E_0 \pm E_I)_i n_i = E, \qquad \sum_i^\infty (E_0 \pm E_I)_i dn_i = 0. \tag{12}$$

Subsequently, the Fermi-Dirac statistics based on ionization energy can be derived as

$$\frac{n_i}{q_i} = \frac{1}{\exp[\mu + \lambda(E_0 \pm E_I)_i] + 1}. \tag{13}$$

By utilizing Eq. (13) and taking $\exp[\mu + \lambda(E \pm E_I)] \gg 1$, one can arrive at the probability function for electrons in an explicit form as

$$f_e = \exp\left[-\mu - \lambda\left(\frac{\hbar^2 \mathbf{k}_0^2}{2m} + E_I\right)\right], \tag{14}$$

Similarly, the probability function for the holes is given by

$$f_h = \exp\left[\mu + \lambda\left(\frac{\hbar^2 \mathbf{k}_0^2}{2m} - E_I\right)\right]. \tag{15}$$

The parameters μ and λ are the Lagrange multipliers. $\hbar = h/2\pi$, h = Planck constant and m is the charge carriers' mass. In the standard FDS, Eqs. (14) and (15) are simply given by, $f_e(\mathbf{k}) = \exp[-\mu - \lambda(\hbar^2\mathbf{k}^2/2m)]$ and $f_h(\mathbf{k}) = \exp[\mu + \lambda(\hbar^2\mathbf{k}^2/2m)]$ respectively.

Subsequently Eq. (11) can be rewritten by employing the 2D density of states' (DOS) derivative, $dn = L^2\mathbf{k}_0 d\mathbf{k}_0/2\pi$, Eqs. (14) and (15), that eventually give

$$n = \frac{L^2}{2\pi}e^{-\mu-\lambda E_I}\int_0^\infty \mathbf{k}_0 \exp\left(-\lambda\frac{\hbar^2\mathbf{k}_0^2}{2m}\right)d\mathbf{k}_0, \quad (16)$$

$$p = \frac{L^2}{2\pi}e^{\mu-\lambda E_I}\int_{-\infty}^0 \mathbf{k}_0 \exp\left(\lambda\frac{\hbar^2\mathbf{k}_0^2}{2m}\right)d\mathbf{k}_0. \quad (17)$$

Note here that E_0 is substituted with $\hbar^2\mathbf{k}_0^2/2m$. n and p are the respective concentrations of electrons and holes. L^2 denotes area in $\mathbf{k}$-space. The respective solutions of Eqs. (16) and (17) are given below

$$e^{\mu+\lambda E_I} = \frac{mL^2}{2n\pi\lambda\hbar^2}, \quad (18)$$

$$e^{\mu-\lambda E_I} = \frac{2p\pi\lambda\hbar^2}{mL^2}, \quad (19)$$

Equations (18) and (19) respectively imply that

$$\mu_e(iFDS) = \mu_e + \lambda E_I, \quad (20)$$

$$\mu_h(iFDS) = \mu_h - \lambda E_I. \quad (21)$$

On the other hand, using Eq. (12), one can obtain

$$E = \frac{L^2\hbar^2}{4m\pi}e^{-\mu-\lambda E_I}\int_0^\infty \mathbf{k}_0^3 \exp\left(\frac{-\lambda\hbar^2\mathbf{k}_0^2}{2m}\right)d\mathbf{k}_0$$
$$= \frac{m}{2\pi}\left(\frac{L}{\lambda\hbar}\right)^2 e^{-\mu-\lambda E_I}. \quad (22)$$

Equation (22), after appropriate substitution with Eq. (18) is compared with the energy of a 2D ideal gas, $E = nk_BT$. Quantitative comparison will eventually leads to $\lambda_{iFDS} = \lambda_{FDS} = 1/k_BT$ where k_B is the Boltzmann constant. The distribution function for electrons and holes can be written explicitly by first denoting $\mu = -E_F$ (Fermi level), $\lambda = 1/k_BT$ and substituting these into Eqs. (14) and (15) will lead one to write

$$f_e(E, E_I) = \exp\left[\frac{E_F - E_I - E}{k_BT}\right]. \quad (23)$$

$$f_h(E, E_I) = \exp\left[\frac{E - E_I - E_F}{k_BT}\right]. \quad (24)$$

Note that Eqs. (20) and (21) simply imply that $\mu_e(iFDS) = \mu(T = 0) + \lambda E_I$ and $\mu_h(iFDS) = \mu(T = 0) - \lambda E_I$. In fact, $\mu(FDS)$ need to be varied accordingly with doping, on the other hand, iFDS captures the same variation due to doping with λE_I in which, $\mu(T = 0)$ is fixed to be a constant (independent of T and doping). Furthermore, using Eqs. (4), (12) and (22), one can obtain

$$E_{iFDS} = \frac{L^2\hbar^2}{4m\pi}e^{-\mu-\lambda E_I}\int_0^\infty \mathbf{k}_0^3 \exp\left(\frac{-\lambda\hbar^2\mathbf{k}_0^2}{2m}\right)d\mathbf{k}_0$$
$$= \frac{L^2\hbar^2}{4m\pi}e^{-\mu}\int_0^\infty \mathbf{k}_0^3 \exp\left(-\frac{\lambda\hbar^2\mathbf{k}_0^2}{2m} - \frac{\lambda\hbar^2\mathbf{k}_\xi^2}{2m}\right)d\mathbf{k}_0$$
$$= \frac{L^2\hbar^2}{4m\pi}e^{-\mu}\int_0^\infty \mathbf{k}^3 \exp\left(-\frac{\lambda\hbar^2\mathbf{k}^2}{2m}\right)d\mathbf{k}$$
$$= E_{FDS}. \quad (25)$$

Eventually, Eq. (25) proves that the total energy of n particles considered in both FDS and iFDS is exactly the same.

3. Heat capacity and its conductivity

Electrons and phonons can be excited to a higher energy levels satisfying the ionization energy based Fermi-Dirac ($f_{iFDS}(E)$) and Bose-Einstein $f_{BES}(E)$ statistics respectively. Therefore, the heat capacity can be explicitly written as

$$\mathcal{C} = \frac{m^*}{\pi\hbar^2}\left[\int_0^\infty (E - E_F - E_I)\frac{\partial f_{iFDS}(E)}{\partial T}dE\right.$$
$$\left. + \int_0^\infty (E - E_F)\frac{\partial f_{BES}(E)}{\partial T}dE\right]. \quad (26)$$

$\hbar = h/2\pi$, h denotes Planck constant, while m^* represents the effective mass. The respective distribution functions for BES and iFDS (using Eq. (4)) are given by $f_{BES}(E) = 1/[\exp\left[(E - E_F)/k_BT\right] - 1] \approx \exp\left[(E_F - E)/k_BT\right]$ and $f_{iFDS}(E) = 1/[\exp\left[(E - E_F + E_I)/k_BT\right] + 1] \approx \exp\left[(E_F - E_I - E)/k_BT\right]$. These approximations

are necessary to avoid the exponential integral function, $\Xi_i(z) = \int_{-z}^{\infty}[e^{-t}/t]dt$, which has a branch cut discontinuity in the complex z plane running from $-\infty$ to 0. Additionally, I highlight that for classical particles satisfying the Maxwell-Boltzmann statistics (MBS), there is no such thing as E_I. Consequently, one should not assume that $\exp[\mu + \lambda(E_{initial\ state} \pm E_I)] \gg 1$ should give the MB distribution function as a classical or a free-electron limit. One can indeed arrive at MBS by first considering the additional constraint, $E_I = 0$ in such cases, where E_{total} now equals to E identical with the standard FDS and MBS. Therefore, the electron's Fermi level, E_F term that contained in $f_{BES}(E)$ corresponds to the phonons' energies above this E_F, in which this E_F does not imply phonons' chemical potential. In other words, phonons with energies $< E_F$ are neglected. In summary, iFDS captures the Fermi liquid ($\xi \neq 0$) rather than the Fermi gas ($V(x) = 0$).

The total heat capacity in Eq. (26) has been written as $\mathcal{C} = \mathcal{C}^e + \mathcal{C}^{ph}$ as a result of the total heat current, $\kappa = -\sum_{\alpha} j_Q^{\alpha}(\nabla T)^{-1} = \sum_{\alpha} \mathcal{C}^{\alpha} v_F^2 \tau_{\nu}/2$. $\alpha = $ electron (e), phonon (ph) and $\nu = e\text{-}e$, $e\text{-}ph$ scattering. v_F denotes the Fermi velocity and k_B is the Boltzmann constant. Importantly, E_I is microscopically defined as [7]

$$\epsilon(0, \mathbf{k}) = 1 + \frac{\mathcal{K}_s^2}{\mathbf{k}^2} \exp\left[\lambda(E_F^0 - E_I)\right]. \qquad (27)$$

$\epsilon(0, \mathbf{k})$ is the static dielectric function, $\mathbf{k}$ and λ are the wavevector and Lagrange multiplier respectively. The E_F^0 denotes the Fermi level at 0 K, while the $\mathcal{K}_s$ represents the Thomas-Fermi screening parameter. Unlike electrical resistivity in YBa$_2$Cu$_3$O$_7$, its 2D heat conductivity is equally strongly influenced by $e\text{-}e$ and $e\text{-}ph$ interactions, hence (after taking $E_F = \frac{1}{2}m^* v_F^2$)

$$\kappa = \tau_{e-e}\mathcal{C}^e \frac{E_F}{m^*} + \tau_{e-ph}\mathcal{C}^{ph} \frac{E_F}{m_{ph}^*}. \qquad (28)$$

The explicit form of Eq. (28) can be obtained after substituting Eq. (26) into Eq. (28) appropriately. The electron-electron scattering rate, $\tau_{e-e}^{-1} = \tau_e^{-1} = AT^2$ while the electron-phonon scattering rate, τ_{e-ph}^{-1} is assumed to be proportional to T^{α} in which $\alpha > 2$. The Fermi-level in Eqs. (26) and (28) implies that the phonons considered here have the thermal energies in the order of or higher than the electrons' Fermi energy which eventually means that these electrons cannot form Fermi gas. In simple words, if the thermal energies of the phonons are less than the electrons' E_F, then these electrons can act as Fermi gas and one may employ the Debye approximation. This is another reason why Debye model works extremely well at intermediate and low temperatures in common metals. However, the phonons' effective mass is equal to the ions reduced mass due to phonons interaction with free-electrons, $1/m_{ph}^* = 1/m_e + 1/m_{ion}$, which

needs to be determined from other techniques, be it theoretical or experimental. Therefore, only the electron's effective mass is highlighted here. In other words, instead of addressing $1/m_{ph}^*$ as the reduced mass of ions, it has been labelled as phonons effective mass so that one can conveniently identify it as the parameter belonging to the phonons' contribution.

4. Resistivity and Hall resistance

The equations of motion (EOM) for charge carriers in ab-planes under the influence of static magnetic ($\mathbf{H}$) and electric fields ($\mathbf{E}$) can be written in an identical fashion as given in Ref. [35], which are given by $m^*[d/dt + 1/\tau_e]v_b = e\mathbf{E}_b + e\mathbf{H}_c v_a$ and $m^*[d/dt + 1/\tau_e]v_a = e\mathbf{E}_a - e\mathbf{H}_c v_b$. The charge, e is defined as negative in the EOM above. Moreover, it is important to realize that the existence of electrons in ab-planes below $T_{crossover}$ are actually holes. The existence of holes in ab-planes was discussed intensively in the Refs. [36, 37, 38]. The subscripts a, b and c represent the axes in a, b and c directions while the subscript ab represents the ab-planes. In a steady state of a static $\mathbf{H}$ and $\mathbf{E}$, $dv_a/dt = dv_b/dt = 0$ and $v_a = 0$ hence one can obtain $\mathbf{E}_a = e\mathbf{H}_c\mathbf{E}_b\tau_e/m^*$. The Hall resistance and current along a- and b-axes are respectively defined as $R_H^{(a)} = \mathbf{E}_a/j_b\mathbf{H}_c$, $j_b = \mathbf{E}_b/\rho$ in which, $\tan\theta_H^{(a)} = \mathbf{E}_a/\mathbf{E}_b$. Parallel to this, $R_H^{(a)} = \tan\theta_H^{(a)}\rho/\mathbf{H}_c$. j_b is the current due to holes motion along b-axis and $\theta_H^{(a)}$ is the Hall angle in ab-planes. Furthermore, one can rewrite $\tan\theta_H^{(a)}$ as $\tan\theta_H^{(a)} = e\mathbf{H}_c/m^*AT^2$, which eventually suggests, $\cot\theta_H^{(a)} \propto T^2$. A is τ_e dependent constant and is independent of T. The 2D resistivity model, $\rho(T)$ is given by [1, 2, 3]

$$\rho(T) = A\frac{\pi\hbar^2}{k_B e^2}T \exp\left[\frac{E_I + E_F}{T}\right]. \qquad (29)$$

Utilizing Eq. (29), one can show that the Hall resistance is given by

$$R_H = \frac{\pi\hbar^2}{m^*Tk_B e} \exp\left[\frac{E_I + E_F}{T}\right]. \qquad (30)$$

Thus, it is clear that R_H is proportional to $1/T$ regardless of the axes. Detailed analysis and diagnosis of Eq. (29) with a wide variety of experimental data are well documented in the Refs. [1, 2, 3]. Optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$ single crystal (A1) obtained from Ref. [39] will be utilized in the following analysis. Equation (29) has been employed to theoretically reproduce (indicated with a solid line in the inset of Fig. 1) the experimental $\rho_{ab}(T)$ by varying the T-independent scattering rate constant, A (7.3×10^{-7} Ω·cm) whereas $E_I + E_F = $

$T_{crossover}$ (T_{cr}) is taken as 0 K, since any optimally doped $YBa_2Cu_3O_7$ gives $T_{cr} \ll T_c$ in which T_{cr} is not observable from the resistivity measurements. I.e., T_{cr} cannot be predicted accurately from the normal state resistivity measurements. On the other hand, the $R_H^{(ab)}(T)$ data and the plot using Eq. (30) are depicted in Fig. 1. Note that $A = A\pi\hbar^2/k_B e^2$ from Eq. (29) and $A_H = \pi\hbar^2/m^* k_B e$ = 347 JKCs^{2}kg^{-1} from Eq. (30). In the latter approximation, $m^* = 50m_0$, m_0 is the rest mass of the electron. In order to accurately fit the experimental $R_H^{(ab)}(T)$ data, the effective mass should be equal to $73m_0$, which in turn gives the charge carriers density as $p = 8 \times 10^{22}$ cm^{-3}, in accordance with the Refs. [3, 17].

5. Lorentz ratio

Lanzara et $al.$ [27] have shown that the e-ph coupling is somewhat inevitable, which has been observed via ARPES technique. Indeed this supports the notion of polaronic effect above T_c in cuprates. One should note that the observation e-ph coupling does not mean that there is a e-ph scattering since normal state $\rho(T)$ measurements thus far failed to reveal any e-ph scattering (strong T-dependence). Actually, this is not because of $\rho(T)$'s blindness, but due to polaronic effect represented by E_I, which gives rise to the effective mass (m^*) of electrons instead of strong T-dependence. The heavier m^* implies the existence of polaronic effect in the normal state of HTSC that also suppresses e-ph scattering but not the e-ph coupling in term of polaronic effect. Similarly, isotope effect (^{18}O, ^{16}O) in cuprates [40, 41, 42] also reinforces the polaronic contribution via e-ph coupling rather than e-ph scattering. In fact, Hofer et $al.$ [40] claimed that m^* reduces towards the optimally doped HTSC. This scenario is consistent with iFDS based models that predicts T_{cr} also reduces towards optimal doping. Simply put, reduced E_I will eventually lead to reduced m^* and consequently the influence of isotope doping on m^* is less effective in optimally doped regime as compared to under doped. The inappropriateness of the e-ph scattering in YBCO$_7$ will be discussed in detail based on the Bloch-Grüneisen formula shortly. From the definition, $\mathcal{L}$ can be written as

$$\mathcal{L} = \frac{\rho}{T}\kappa = \kappa A \frac{\pi\hbar^2}{k_B e^2} \exp\left[\frac{E_I + E_F}{T}\right]. \quad (31)$$

Interestingly, Sutherland et $al.$ [43] have reported only a slight increase (upward deviation) in ab-plane's heat conductivity with phonon contribution ($\kappa_{ab}^{100K}/\kappa_{ab}^{300K}$ ≤ 1.3) above critical temperature (T_c) for overdoped YBCO. Their results will be used to discuss the accuracy of Eqs. (28) and (31) to capture the experimental data.

6. e-ph scattering in resistivity

Firstly, the Bloch-Grüneisen (BG) formula will be revisited in order to rule out the e-ph scattering in the normal state of YBCO$_7$. Recall that the polaronic effect that arises from the E_I based Fermi-Dirac statistics (iFDS) has been successful to explain and predict the evolution of resistivity with doping and to enumerate the minimum valence state of multivalent dopants in HTSC, ferromagnets and recently in doped-ferroelectrics. But iFDS does not reveal the inadequacy of the free e-ph scattering directly (only indirectly). Basically, according to the e-ph scattering, the electrons from Ba^{2+} and Sr^{2+} as in Y(Ba$_{1-x}$Sr$_x$)$_2$Cu$_3$O$_7$ has the same effect on transport measurements while iFDS points out that the kinetic energy (KE) of the electrons from Ba^{2+} is not equal with the KE of the electrons from Sr^{2+}, which gives rise to significant changes of resistivity with small doping. Again, if one assumes KE (Ba^{2+}) = KE (Sr^{2+}), then the theory of the e-ph scattering is indeed applicable due to isotropy in KE (all the free electrons have an identical KE, which eventually defines the Fermi surfaces). Hence, to further evaluate the incompatibility of the e-ph scattering in YBCO$_7$, the BG formula [44] stated in Eq. 32 is employed to plot the T-dependence of $\rho(T)$ (assuming $\tau_{e-ph}(3D) \propto \tau_{e-ph}(2D)$) and $\mathcal{L}(T)$.

$$\rho_{BG} = \lambda_{tr}\frac{128\pi m^* k_B T^5}{ne^2\Theta_D^4} \int\limits_0^{\Theta_D/2T} \frac{x^5}{\sinh^2 x}dx. \quad (32)$$

λ_{tr} = electron-phonon coupling constant, m^* = average effective mass of the occupied carrier states, Θ_D = Debye temperature, n = free electrons concentration. The $\mathcal{L}(T)$ can be simply written as

$$\mathcal{L}_{BG} = \kappa\lambda_{tr}\frac{128\pi m^* k_B T^4}{ne^2\Theta_D^4} \int\limits_0^{\Theta_D/2T} \frac{x^5}{\sinh^2 x}dx. \quad (33)$$

7. Analysis

Figure 2 a) and b) depict the T-dependence of $\rho(T)$ (Eq. (32)) and $\mathcal{L}(T)$ respectively. The $\mathcal{L}(T)$ based on BG's approach after incorporating the experimental κ are indicated with $\triangle$ ($\Theta_D = 200$ K), $\circ$ ($\Theta_D = 300$ K), and $\square$ ($\Theta_D = 350$ K). On the other hand, the experimental and iFDS based theoretical plots (Eqs. (28), (29) and (31)) are shown with $\bullet$ and a solid line, respectively in Fig. 2 b). Note that in Eq. (28), $\alpha = 3$ is used complying with the earlier assumption of $T^{\alpha>2}$. This value is reasonable since α in the free e-ph scattering of conventional metals are known to vary between 3 and 5, depending on

T's range that can be verified from Eq. (32). The experimental $\mathcal{L}(T)$ is obtained from the resistivity [45] and heat conductivity [43] measurements of optimally doped YBCO.

The inverse proportionality of the theoretically determined κ with T from Eq. (28) is understandable since the electrical conductivity is proportional to $1/T$ and there are phonon contribution as well. As a result of this, $\mathcal{L}(T)$ is also inversely proportional to T. It is not possible to evaluate Eq. (28) quantitatively due to the unknown magnitudes of E_I, E_F, m^*_{ph} and A_{e-ph}. However, the measured κ in the normal state of YBCO hardly shows strong T dependence [43] indicating the existence of some not-yet-known physical phenomena, which complicates our understanding of HTSC generally. Anyhow, by using the experimentally determined κ, one can verify the accuracy of the resistivity equations (between Eq. (29) and (32)). The former equation is entirely based on e-e scattering while the latter contains the essential e-ph scattering mechanism. To this end, the lorentz ratio based on iFDS (Eq. (31)) and BG (Eq. (33)) are computed using the almost T independent or experimental κ.

The iFDS model reproduces the T dependence trend, remarkably identical with the experimental data as opposed to the BG's approach. Both iFDS and BG models with the experimental κ have been plotted in Fig. 2 b), in which the latter model is plotted at different Θ_D. Eventually, one can convincingly state that e-ph scattering mechanism is significantly negligible in the electrical resistance measurements. The plot that corresponds to Eq. (31) with experimental κ is obtained using $E_I + E_F = 10$ K, (which is less than T_c as a result of optimal or over doping) and experimental κ that eventually give $A = 1 \times 10^{-8}$ $\Omega \cdot$cm. This magnitude is remarkably identical with the optimally doped crystalline YBCO sample of Hagen *et al.* [19] and Leridon *et al.* [45] that have been calculated ($A_{Hagen,Lerridon} = (1.1, 1.4) \times 10^{-8}$ $\Omega \cdot$cm) and reported in the Refs. [2, 21]. Importantly, even though Eq. (32) can be shown to capture the experimental T-linear property of $\rho(T)$, but it also fails to explain the T_{cr} above T_c for slightly under doped HTSC. T_{cr} is the T where $\rho(T)$ deviates upward exponentially, which has been well explained [1, 2, 3] via E_I in Eq. (29).

8. Conclusions

In conclusion, iFDS based electrical resistivity (with e-e scattering rate only) and heat conductivity (with both e-e and e-ph scattering rate) models have been utilized to tackle the T dependence of Lorentz ratio in optimally doped YBa$_2$Cu$_3$O$_7$. The computed $\mathcal{L}(T)$ with experimental κ overwhelmingly suggests that Bloch-Grüneisen formula or the inclusion of e-ph scattering in the electrical resistivity is not suitable, at least for YBa$_2$Cu$_3$O$_7$. On the other hand, e-ph scattering contributes significantly in heat conductivity that eventually gives a reasonably acceptable picture for the experimental heat conductivity and Lorentz ratio. Additionally, the spin Pseudogap phenomenon have been omitted throughout so as to avoid its inconclusive interpretations. Apart from that, the magnitudes of the T-independent scattering rate constant, effective mass and the charge carriers density are all in the acceptable range, complying with other optimally doped YBCO single crystals as computed previously.

FIG. 1: Experimental $R_H^{(ab)}(T)$ and $\rho_{ab}(T)$ (inset) data points for YBa$_2$Cu$_3$O$_{7-\delta}$ single crystal (A1) have been fitted using Eqs. (30) and (29) respectively. The former equation is computed with two m^*s namely, $50m_0$ and $73m_0$ while the resistivity is calculated with $A = 7.3 \times 10^{-7}$ $\Omega \cdot$cm.

FIG. 2: a) Shows the BG resistivity, $\rho(T)$ plots above 90 K for $\Theta_D = 350$, 300 and 200 K. Whereas, b) depicts the theoretical plots for the BG Lorentz ratio, $\mathcal{L}_{BG}$ above 90 K with experimental heat conductivity (κ) using Eq. (33) with the Debye T, $\Theta_D = 350$, 300 and 200 K. The calculated $\mathcal{L}(T)$ with Eq. (31) using experimental κ is also plotted with $\diamond$ in b). The theoretical solid line in b) satisfies iFDS based models namely, Eqs. (28), (29) and (31) with $\alpha = 3$. The experimental plots indicated with $\bullet$ is obtained from the data combined from Leridon *et al.* [45] and Sutherland *et al.* [43].

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a

Debye T = 350 K
Debye T = 200 K
Debye T = 300 K

2.9

ρ (arb. units)

0

90   **T (K)**   110   130

b

◇ Eq. (6), κ = exptl.
— Eq. (6)

16

L (WΩK^{-2}) X 10^{-8}

350 K ⎫
200 K ⎬ κ = exptl.
300 K ⎭
● YBCO(7) [43,45]

5

90   **T (K)**   110   130